Challenging Dogmas: What is inside a Hydrogen Bond?

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Hydrogen bond directionality in the water dimer is explained based on symmetry-adapted intermolecular perturbation theory, SAPT [1], which directly separates the intermolecular interaction energy into four physically interpretable components: electrostatics, exchange-repulsion, dispersion, and induction. Analysis of these four main contributions to the binding energy allows a deeper understanding of the dominant factors ruling the mutual arrangement of the two monomers. A preference for the linear configuration is shown to be due to a subtle interplay of all the four energy components. While the first-order terms, electrostatic and exchange-repulsion, almost perfectly cancel each other near the equilibrium geometry of the dimer, the importance of the second and higher-order terms, induction and dispersion, becomes evident.

[1] B. Jeziorski, K. Szalewicz, R. Moszynski, *Chem. Rev.*, **1994**, *94*, 1887-1930.